



DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1a. AD-A237 461			1b. RESTRICTIVE MARKINGS none	
2a. 			3. DISTRIBUTION/AVAILABILITY OF REPORT unlimited	
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE				
4. PERFORMING ORGANIZATION REPORT NUMBER(S)			5. MONITORING ORGANIZATION REPORT NUMBER(S)	
6a. NAME OF PERFORMING ORGANIZATION California Institute of Technology		6b. OFFICE SYMBOL (if applicable)	7a. NAME OF MONITORING ORGANIZATION Office of Naval Research	
6c. ADDRESS (City, State, and ZIP Code) Mail Code: 164-30 Pasadena, CA 91125		7b. ADDRESS (City, State, and ZIP Code) Code 1113PO (H. Guard) 800 N. Quincy Street Arlington, VA 22217-5000		
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Office of Naval Research		8b. OFFICE SYMBOL (if applicable) ONR	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N00014-88-K-0259	
8c. ADDRESS (City, State, and ZIP Code) 800 N. Quincy Street Arlington, VA 22217-5000		10. SOURCE OF FUNDING NUMBERS		
		PROGRAM ELEMENT NO. 6153 N	PROJECT NO. 413p006	TASK NO. WORK UNIT ACCESSION NO.
11. TITLE (Include Security Classification) New Synthetic Receptor Derived from Bridged Anthracenes. unclassified				
12. PERSONAL AUTHOR(S) Dennis A. Dougherty				
13a. TYPE OF REPORT Final Technical	13b. TIME COVERED FROM 3/1/88 to 12/31/90	14. DATE OF REPORT (Year, Month, Day) 91 May 29	15. PAGE COUNT 4	
16. SUPPLEMENTARY NOTATION				
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP	SUB-GROUP		
19. ABSTRACT (Continue on reverse if necessary and identify by block number)				
				
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION	
22a. NAME OF RESPONSIBLE INDIVIDUAL Harold Guard			22b. TELEPHONE (Include Area Code) 202-696-4409	22c. OFFICE SYMBOL

OFFICE OF NAVAL RESEARCH

Grant No.:N00014-88-K-0259

R&T Code:413p006

Final Technical Report

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
by	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

New Synthetic Receptor Derived from Bridged Anthracenes

by

Dennis A. Dougherty

Division of Chemistry and Chemical Engineering
California Institute of Technology
Pasadena, CA 91125

May 31, 1991

Reproduction in whole, or in part is permitted for any purpose of the United States Government.

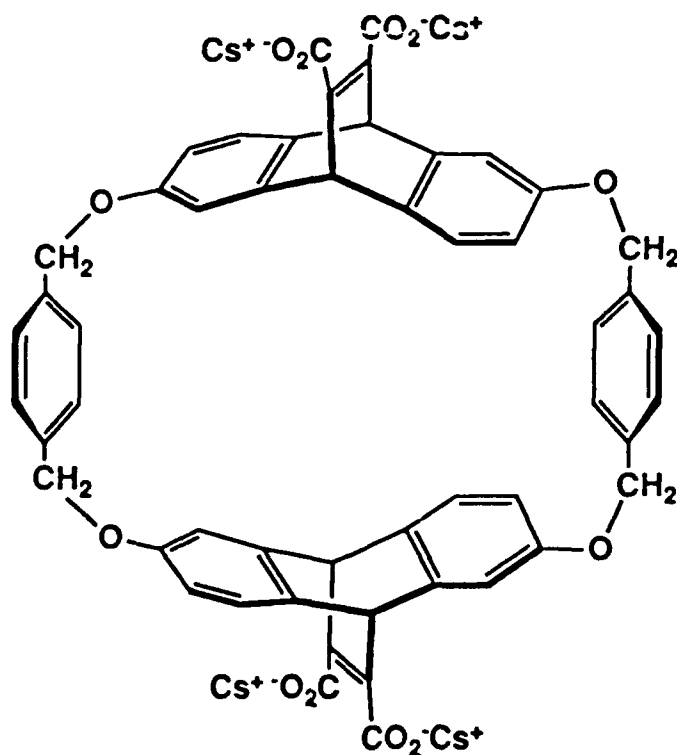
This document has been approved for public release and sale: its distribution is unlimited.

91-03715


FINAL TECHNICAL REPORT
ONR CONTRACT N00014-88-K-0259

Dennis A. Dougherty
Division of Chemistry & Chemical Engineering
California Institute of Technology
Pasadena, CA 91125

The major goal of the present contract was to develop new insights into the forces responsible for the association of organic molecules so often seen in biological systems (eg., enzyme-substrate, antibody-antigen, neuroreceptor-neurotransmitter interactions). To this end, a series of water-soluble organic molecules with well-defined hydrophobic binding sites was prepared, and the binding characteristics of several structures were evaluated.



a typical receptor of the type developed in the present work

The most significant discovery of the investigations was the demonstration of the importance of the "cation- π " (or, alternatively, "ion-dipole") interaction in producing tight, oriented binding of a wide variety of "onium" type guests. High

field NMR was the primary tool used to establish the cation- π interaction as a potent force for binding in both aqueous (technical report number 1) and organic media (technical report number 2). In addition, detailed studies revealed the primarily enthalpic nature of the phenomenon and the dangers of overly simplified analyses of binding data (technical report number 3). It seems quite likely that similar binding forces are of critical importance in a variety of biological receptors, especially many that are involved in several aspects of neurochemistry, and future efforts will seek to strengthen this connection.

In addition, the cation- π interaction has been exploited to develop a novel catalytic system (technical report number 4). It was demonstrated that a certain type of alkylation chemistry, in which a partial positive charge is developed in the transition state, is substantially accelerated by our synthetic receptors. The system is truly catalytic, exhibiting turnover and appropriate competitive inhibition behaviors. This is a novel example of taking a binding force that was discovered in "ground state" systems and using it to preferentially bind transition states. Future work will seek to expand upon and exploit this concept to produce powerful catalysts for useful organic transformation.

PUBLICATIONS PRODUCED

"Hydrophobic" Binding of Water-Soluble Guests by High- Symmetry, Chiral Hosts. An Electron-Rich Receptor Site with a General Affinity for Quaternary Ammonium Compounds and Electron- Deficient π Systems. M.A. Petti, T.J. Shepodd, R.E. Barrans, Jr., and D.A. Dougherty, *J. Am. Chem. Soc.* 1988, 110, 6825-6840.

Ion-Dipole Effect as a Force for Molecular Recognition in Organic Media. D.A. Stauffer and D.A. Dougherty, *Tetrahedron Lett.* 1988, 29, 6039-6042.

Biomimetic Catalysis of an S_N2 Reaction Resulting from a Novel Form of Transition-State Stabilization. D.A. Stauffer, R.E. Barrans, Jr., and D.A. Dougherty, *Angew. Chem. Int. Ed. Engl.* 1990, 29, 915-918.

Concerning the Thermodynamics of Molecular Recognition in Aqueous and Organic Media. Evidence for Significant Heat Capacity Effects. D.A. Stauffer, R.E. Barrans, Jr., and D.A. Dougherty, *J. Org. Chem.*, 1990, 55, 2762-2767.

TECHNICAL REPORTS

Technical Report No.1 - "'Hydrophobic' Binding of Water-Soluble Guests by High-Symmetry, Chiral Hosts. An Electron-Rich Receptor Site with a General Affinity for Quarternary Ammonium Compounds and Electron-Deficient π Systems." M.A. Petti, T.J. Shepodd, R.E. Barrans, Jr., and D.A. Dougherty.

Technical Report No. 2 - "Ion-Dipole Effect as a Force for Molecular Recognition in Organic Media." D.A. Stauffer and D.A. Dougherty.

Technical Report No. 3 - Concerning the Thermodynamics of Molecular Recognition in Aqueous and Organic Media. Evidence for Significant Heat Capacity Effects." D.A. Stauffer, R.E. Barrans, Jr., and D.A. Dougherty

Technical Report No. 4 - "Biomimetic Catalysis of an S_N2 Reaction Resulting from a Novel Form of Transition-State Stabilization." D.A. Stauffer, R.E. Barran, Jr., and D.A. Dougherty.